2-Hydroxy-3-methoxybenzaldehyde

148-53-8 | DTXSID5022011

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 1.29e-03 mmHg

Global applicability domain: Inside

Local applicability domain index: 6.79e-01

Confidence level: 3.95e-01

Nearest Neighbors from the Training Set

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Butyl phenyl ether
Measured: 1.08e-03
Predicted: 5.92e-01

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2,6-Diethylaniline
Measured: 1.59e-05
Predicted: 2.02e-02

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4-(2,4-Dinitroanilino)phenol
Measured: 3.43e-02
Predicted: 1.31e-11

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2-Methoxyprop-1-ene
Measured: 8.46e-02
Predicted: 474